



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:40 AM UTC

PDB ID : 3DRO / pdb_00003dro
Title : Crystal structure of the HIV-1 Cross Neutralizing Antibody 2F5 in complex with gp41 Peptide ELLELDKWASLWN grown in ammonium sulfate
Authors : Julien, J.-P.; Bryson, S.; Pai, E.F.
Deposited on : 2008-07-11
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

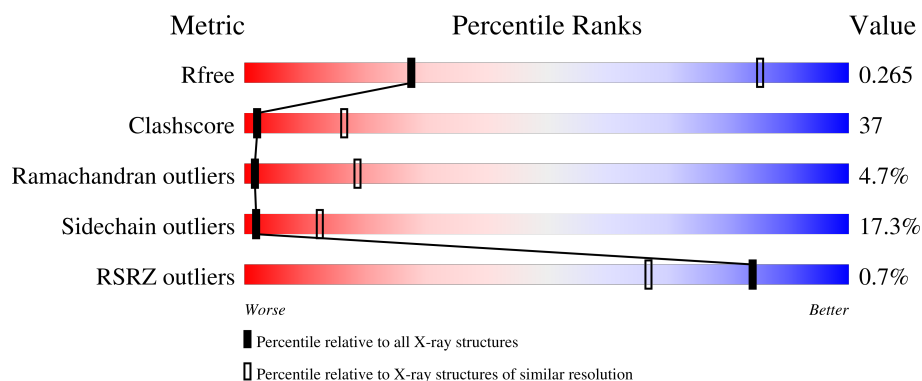
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	 49% 38% 11% •
2	B	235	 39% 37% 14% • 8%
3	P	13	 23% 15% 15% 46%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3321 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2F5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1637	1022	280	331	4			

- Molecule 2 is a protein called 2F5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1623	1030	274	313	6			

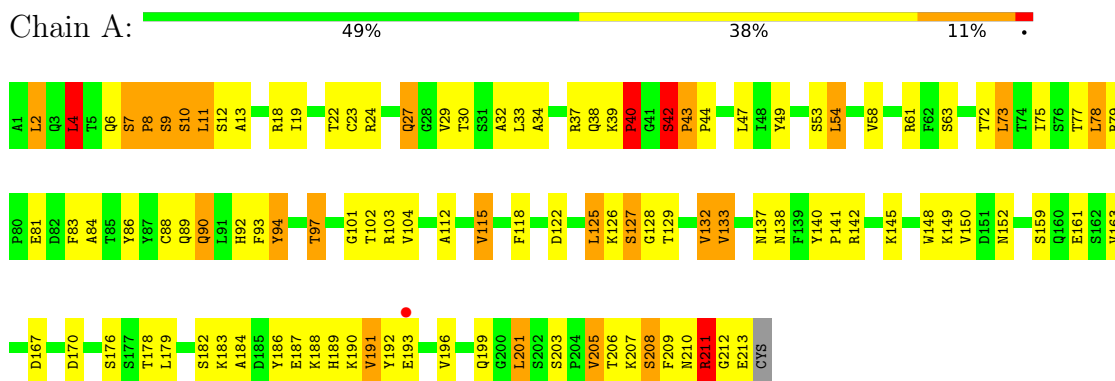
- Molecule 3 is a protein called ELLELDKWASLWN gp41 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	7	Total	C	N	O	0	0	0
			61	41	9	11			

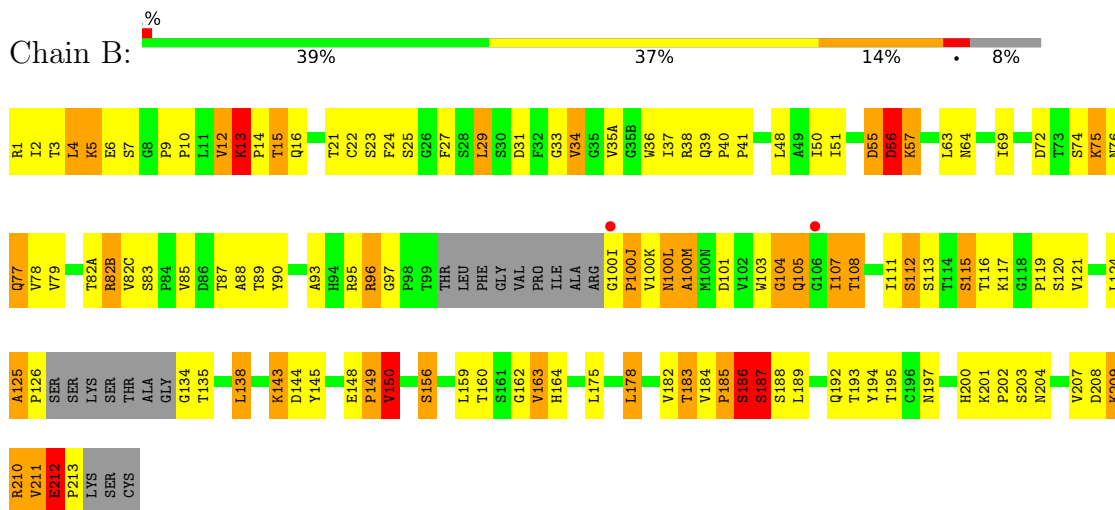
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

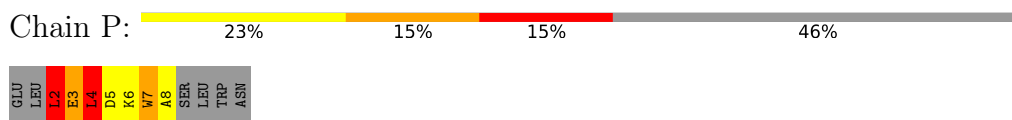
• Molecule 1: 2F5 Fab light chain



• Molecule 2: 2F5 Fab heavy chain



• Molecule 3: ELLELDKWASLWN gp41 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.90Å 76.50Å 93.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.96 – 3.90 16.96 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.6 (16.96-3.90) 92.3 (16.96-3.90)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 3.50Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.263 0.227 , 0.265	Depositor DCC
R_{free} test set	306 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3321	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.59	0/1674	1.17	21/2276 (0.9%)
2	B	0.59	0/1662	1.31	23/2273 (1.0%)
3	P	1.07	0/62	2.96	7/83 (8.4%)
All	All	0.60	0/3398	1.29	51/4632 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	P	0	1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	GLU	N-CA-C	14.16	131.21	108.41
3	P	2	LEU	N-CA-C	12.36	145.62	111.00
2	B	212	GLU	N-CA-C	11.34	118.43	108.22
3	P	4	LEU	N-CA-C	9.51	122.11	110.41
2	B	56	ASP	N-CA-C	-9.24	95.43	109.94
1	A	127	SER	N-CA-C	-8.49	92.70	110.80
2	B	55	ASP	N-CA-C	8.39	123.07	111.74
2	B	55	ASP	CA-C-N	-8.37	106.66	122.73
2	B	55	ASP	C-N-CA	-8.37	106.66	122.73
2	B	211	VAL	N-CA-C	7.99	119.68	107.78
2	B	207	VAL	N-CA-C	7.95	120.59	107.24
2	B	104	GLY	N-CA-C	-7.94	98.96	112.30
2	B	101	ASP	N-CA-C	7.84	120.92	111.82
2	B	56	ASP	N-CA-CB	7.76	124.12	110.07
1	A	94	TYR	N-CA-C	-7.59	100.50	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	GLU	N-CA-CB	-7.55	98.21	110.21
1	A	4	LEU	N-CA-C	-7.43	94.97	110.80
2	B	135	THR	N-CA-C	-7.25	98.13	109.72
1	A	42	SER	N-CA-C	7.21	125.73	109.81
1	A	137	ASN	N-CA-C	6.81	120.33	109.24
1	A	97	THR	N-CA-C	6.76	120.42	109.40
2	B	162	GLY	N-CA-C	-6.75	106.66	114.69
1	A	209	PHE	N-CA-C	-6.59	99.02	109.23
3	P	7	TRP	N-CA-C	6.57	120.89	113.01
1	A	43	PRO	N-CA-C	6.45	118.57	110.70
2	B	13	LYS	N-CA-C	6.33	118.05	110.07
2	B	64	ASN	N-CA-C	6.33	118.70	111.11
2	B	100(L)	ASN	N-CA-C	6.29	118.58	110.65
1	A	196	VAL	N-CA-C	6.22	116.88	108.17
2	B	207	VAL	N-CA-CB	-6.15	104.22	112.10
2	B	120	SER	N-CA-C	-6.02	99.38	109.07
1	A	128	GLY	N-CA-C	5.94	123.80	115.43
3	P	2	LEU	CA-C-N	5.83	130.17	122.42
3	P	2	LEU	C-N-CA	5.83	130.17	122.42
1	A	40	PRO	N-CA-C	5.78	124.37	112.47
1	A	211	ARG	N-CA-C	5.74	123.02	110.80
1	A	9	SER	N-CA-C	5.62	120.46	111.81
1	A	212	GLY	N-CA-C	5.60	126.45	113.18
1	A	115	VAL	N-CA-C	5.59	116.35	108.36
2	B	143	LYS	N-CA-C	5.58	119.07	110.42
1	A	210	ASN	N-CA-C	-5.53	99.71	108.73
2	B	12	VAL	N-CA-C	5.49	116.65	108.46
2	B	125	ALA	N-CA-C	5.48	119.03	109.82
1	A	191	VAL	CB-CA-C	-5.42	104.74	111.08
2	B	150	VAL	N-CA-C	-5.37	100.62	108.99
1	A	182	SER	N-CA-C	-5.31	101.04	109.96
1	A	43	PRO	CA-C-N	5.29	125.23	119.78
1	A	43	PRO	C-N-CA	5.29	125.23	119.78
1	A	12	SER	N-CA-C	-5.23	98.50	107.23
2	B	82(C)	VAL	CB-CA-C	-5.17	105.90	111.59
2	B	78	VAL	N-CA-C	-5.14	100.80	108.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	2	LEU	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1637	0	1583	106	0
2	B	1623	0	1630	128	0
3	P	61	0	59	21	0
All	All	3321	0	3272	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:ARG:HG3	2:B:2:ILE:H	0.99	1.12
1:A:7:SER:HB3	1:A:8:PRO:HD2	1.24	1.09
2:B:96:ARG:HB2	2:B:100(K):VAL:HA	1.36	1.07
1:A:7:SER:HB2	1:A:22:THR:OG1	1.57	1.03
1:A:7:SER:HB3	1:A:8:PRO:CD	1.89	1.01
2:B:1:ARG:CG	2:B:2:ILE:H	1.73	1.00
1:A:7:SER:CB	1:A:8:PRO:HD2	1.96	0.95
1:A:103:ARG:HH22	1:A:142:ARG:HD2	1.29	0.95
1:A:38:GLN:O	1:A:84:ALA:HB1	1.67	0.95
2:B:1:ARG:HG3	2:B:2:ILE:N	1.82	0.94
2:B:150:VAL:HG23	2:B:200:HIS:HB2	1.49	0.93
1:A:125:LEU:O	1:A:183:LYS:HD2	1.68	0.92
1:A:11:LEU:HB2	1:A:104:VAL:HG22	1.50	0.91
1:A:42:SER:CB	1:A:43:PRO:HD2	2.04	0.87
2:B:125:ALA:HB1	2:B:126:PRO:HD2	1.59	0.84
3:P:4:LEU:N	3:P:4:LEU:HD23	1.96	0.80
2:B:13:LYS:HG3	2:B:113:SER:HA	1.63	0.79
1:A:61:ARG:CZ	1:A:79:ARG:HG3	2.13	0.78
1:A:103:ARG:HH22	1:A:142:ARG:CD	1.96	0.78
1:A:11:LEU:HB3	1:A:104:VAL:HG13	1.64	0.78
1:A:42:SER:HB3	1:A:43:PRO:HD2	1.63	0.78
1:A:6:GLN:NE2	1:A:102:THR:N	2.31	0.77
1:A:132:VAL:HG13	1:A:179:LEU:HB3	1.67	0.77
2:B:96:ARG:CB	2:B:100(K):VAL:HA	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100(J):PRO:C	2:B:100(L):ASN:H	1.91	0.76
2:B:138:LEU:HB2	2:B:211:VAL:HG11	1.66	0.76
2:B:13:LYS:CG	2:B:113:SER:HA	2.15	0.76
2:B:14:PRO:O	2:B:15:THR:HB	1.86	0.75
1:A:7:SER:O	1:A:8:PRO:C	2.30	0.74
1:A:90:GLN:HE22	1:A:93:PHE:H	1.36	0.73
2:B:31:ASP:HB2	2:B:34:VAL:HG21	1.72	0.72
2:B:83:SER:OG	2:B:85:VAL:HG22	1.89	0.71
1:A:193:GLU:HB3	1:A:208:SER:HB3	1.71	0.71
2:B:100(L):ASN:O	2:B:100(M):ALA:HB2	1.89	0.71
1:A:4:LEU:HA	1:A:24:ARG:O	1.91	0.71
1:A:42:SER:CB	1:A:43:PRO:CD	2.69	0.70
2:B:150:VAL:HG23	2:B:200:HIS:CB	2.21	0.70
2:B:96:ARG:HG3	2:B:100(J):PRO:O	1.92	0.69
1:A:126:LYS:O	1:A:126:LYS:HG2	1.91	0.69
2:B:178:LEU:C	2:B:178:LEU:HD12	2.18	0.68
3:P:2:LEU:C	3:P:2:LEU:HD23	2.18	0.68
1:A:90:GLN:NE2	1:A:92:HIS:H	1.90	0.67
2:B:15:THR:O	2:B:82(B):ARG:HA	1.95	0.66
2:B:14:PRO:HD2	2:B:113:SER:HB3	1.78	0.66
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.78	0.66
1:A:159:SER:HA	1:A:178:THR:O	1.96	0.66
2:B:125:ALA:HB2	2:B:211:VAL:HG13	1.78	0.65
2:B:4:LEU:HA	2:B:24:PHE:HA	1.78	0.65
1:A:42:SER:HB2	1:A:43:PRO:HD2	1.78	0.65
1:A:184:ALA:O	1:A:188:LYS:HG2	1.97	0.65
3:P:4:LEU:N	3:P:4:LEU:CD2	2.60	0.65
2:B:125:ALA:HB1	2:B:126:PRO:CD	2.27	0.65
1:A:7:SER:HB2	1:A:22:THR:HG1	1.61	0.64
1:A:189:HIS:O	1:A:211:ARG:NH2	2.30	0.64
1:A:93:PHE:CE1	3:P:4:LEU:HD22	2.32	0.63
1:A:29:VAL:HG23	1:A:29:VAL:O	1.97	0.63
1:A:126:LYS:O	1:A:126:LYS:CG	2.46	0.62
2:B:144:ASP:HB3	2:B:175:LEU:HD13	1.80	0.62
2:B:14:PRO:O	2:B:15:THR:CB	2.48	0.62
1:A:42:SER:HB3	1:A:43:PRO:CD	2.28	0.62
1:A:6:GLN:NE2	1:A:101:GLY:C	2.57	0.62
2:B:111:ILE:HD12	2:B:111:ILE:N	2.16	0.61
2:B:38:ARG:HD2	2:B:90:TYR:CE2	2.35	0.61
2:B:97:GLY:C	2:B:100(K):VAL:HG12	2.26	0.61
2:B:183:THR:HG23	2:B:183:THR:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:O	2:B:107:ILE:HG23	1.99	0.61
2:B:163:VAL:O	2:B:164:HIS:CD2	2.55	0.60
1:A:189:HIS:H	1:A:211:ARG:NH2	2.00	0.60
1:A:11:LEU:CD2	1:A:19:ILE:HD12	2.31	0.60
1:A:32:ALA:HA	2:B:100(L):ASN:OD1	2.02	0.59
2:B:100(K):VAL:HG21	3:P:7:TRP:CD1	2.37	0.59
2:B:184:VAL:HG11	2:B:194:TYR:CE1	2.37	0.59
1:A:103:ARG:NH2	1:A:142:ARG:CD	2.65	0.59
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.84	0.59
2:B:100(L):ASN:O	2:B:100(M):ALA:CB	2.51	0.58
1:A:187:GLU:C	1:A:211:ARG:NH2	2.61	0.58
3:P:2:LEU:CG	3:P:3:GLU:N	2.63	0.58
2:B:24:PHE:CZ	2:B:29:LEU:HD22	2.37	0.58
2:B:188:SER:HB2	2:B:192:GLN:HB2	1.85	0.58
3:P:2:LEU:CG	3:P:3:GLU:H	1.96	0.58
2:B:24:PHE:HZ	2:B:29:LEU:HD22	1.69	0.57
2:B:56:ASP:C	2:B:57:LYS:HG3	2.28	0.57
1:A:63:SER:O	1:A:73:LEU:HD23	2.04	0.57
2:B:183:THR:O	2:B:183:THR:CG2	2.53	0.57
1:A:4:LEU:HD21	1:A:23:CYS:SG	2.45	0.57
2:B:12:VAL:O	2:B:111:ILE:HA	2.05	0.57
1:A:189:HIS:H	1:A:211:ARG:HH21	1.53	0.56
2:B:186:SER:O	2:B:187:SER:C	2.48	0.56
3:P:2:LEU:HD23	3:P:3:GLU:N	2.20	0.56
2:B:195:THR:HA	2:B:210:ARG:HA	1.86	0.56
2:B:75:LYS:O	2:B:76:ASN:HB2	2.04	0.56
2:B:2:ILE:HG23	2:B:27:PHE:CD2	2.40	0.56
1:A:6:GLN:HA	1:A:23:CYS:HA	1.85	0.56
1:A:54:LEU:CD2	1:A:58:VAL:HB	2.35	0.56
2:B:37:ILE:N	2:B:37:ILE:HD12	2.21	0.56
3:P:3:GLU:O	3:P:3:GLU:HG3	2.06	0.56
2:B:100(K):VAL:CG2	3:P:7:TRP:CD1	2.89	0.55
1:A:32:ALA:HB3	1:A:92:HIS:HB2	1.88	0.55
1:A:6:GLN:HE22	1:A:102:THR:N	2.04	0.55
2:B:126:PRO:HD3	2:B:138:LEU:HB3	1.88	0.55
2:B:38:ARG:HB3	2:B:48:LEU:HD11	1.89	0.55
2:B:211:VAL:C	2:B:212:GLU:HG3	2.31	0.55
1:A:6:GLN:HE21	1:A:102:THR:CB	2.20	0.55
1:A:93:PHE:CD1	3:P:4:LEU:HD22	2.42	0.55
3:P:3:GLU:C	3:P:3:GLU:OE1	2.49	0.55
2:B:23:SER:OG	2:B:77:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLY:C	2:B:100(K):VAL:CG1	2.80	0.55
1:A:10:SER:HA	1:A:103:ARG:O	2.07	0.55
1:A:2:LEU:CD2	1:A:90:GLN:HG2	2.37	0.54
2:B:36:TRP:O	2:B:48:LEU:HB2	2.08	0.54
1:A:11:LEU:HD23	1:A:19:ILE:CD1	2.38	0.54
2:B:1:ARG:CG	2:B:2:ILE:N	2.44	0.54
1:A:125:LEU:HD22	1:A:183:LYS:HG3	1.89	0.54
2:B:5:LYS:HG3	2:B:6:GLU:N	2.22	0.54
2:B:82(A):THR:O	2:B:82(B):ARG:C	2.50	0.54
1:A:6:GLN:HE21	1:A:102:THR:N	2.05	0.53
2:B:212:GLU:CB	2:B:213:PRO:CD	2.86	0.53
1:A:201:LEU:HD13	1:A:205:VAL:HG13	1.91	0.53
2:B:186:SER:O	2:B:188:SER:N	2.42	0.53
1:A:7:SER:O	1:A:8:PRO:O	2.25	0.53
1:A:118:PHE:HD2	1:A:133:VAL:HG22	1.74	0.53
2:B:184:VAL:HG11	2:B:194:TYR:CZ	2.44	0.52
1:A:2:LEU:HD21	1:A:90:GLN:HG2	1.92	0.52
2:B:143:LYS:HG2	2:B:144:ASP:OD2	2.10	0.52
2:B:200:HIS:CD2	2:B:202:PRO:HD2	2.43	0.52
1:A:89:GLN:HA	1:A:97:THR:O	2.10	0.52
2:B:111:ILE:N	2:B:111:ILE:CD1	2.73	0.52
3:P:4:LEU:HD23	3:P:4:LEU:H	1.75	0.52
1:A:112:ALA:HB1	1:A:201:LEU:HD21	1.92	0.52
2:B:97:GLY:N	2:B:100(K):VAL:HG12	2.24	0.51
1:A:61:ARG:CZ	1:A:79:ARG:CG	2.88	0.51
2:B:31:ASP:HB2	2:B:34:VAL:CG2	2.39	0.51
1:A:112:ALA:HB1	1:A:201:LEU:CD2	2.41	0.51
1:A:132:VAL:HG22	1:A:148:TRP:CH2	2.46	0.51
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.46	0.50
2:B:212:GLU:CB	2:B:213:PRO:HD2	2.41	0.50
1:A:11:LEU:N	1:A:103:ARG:O	2.44	0.50
2:B:24:PHE:HB2	2:B:27:PHE:CE2	2.46	0.50
2:B:22:CYS:O	2:B:77:GLN:HA	2.11	0.50
1:A:32:ALA:O	1:A:90:GLN:HA	2.12	0.50
2:B:103:TRP:C	2:B:104:GLY:O	2.51	0.49
1:A:11:LEU:HD23	1:A:19:ILE:HD12	1.94	0.49
1:A:73:LEU:C	1:A:73:LEU:HD22	2.38	0.49
1:A:75:ILE:HG21	1:A:78:LEU:HD23	1.95	0.49
1:A:161:GLU:HA	1:A:176:SER:O	2.12	0.49
2:B:41:PRO:HD3	2:B:87:THR:O	2.13	0.49
3:P:2:LEU:C	3:P:2:LEU:CD2	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:GLU:OE1	3:P:4:LEU:N	2.46	0.49
1:A:186:TYR:O	1:A:192:TYR:OH	2.29	0.49
1:A:11:LEU:HD21	1:A:19:ILE:HB	1.94	0.49
2:B:96:ARG:CG	2:B:100(K):VAL:HA	2.43	0.48
1:A:2:LEU:HD13	1:A:93:PHE:CD2	2.47	0.48
2:B:89:THR:HA	2:B:108:THR:HA	1.95	0.48
2:B:138:LEU:HB2	2:B:211:VAL:CG1	2.40	0.48
2:B:51:ILE:HB	2:B:69:ILE:HD13	1.96	0.48
1:A:167:ASP:HB3	1:A:170:ASP:OD2	2.13	0.48
2:B:96:ARG:HG3	2:B:100(K):VAL:HA	1.96	0.48
2:B:111:ILE:O	2:B:112:SER:HB2	2.14	0.47
2:B:39:GLN:C	2:B:88:ALA:HB1	2.39	0.47
2:B:4:LEU:HD12	2:B:4:LEU:H	1.78	0.47
2:B:195:THR:HG23	2:B:210:ARG:N	2.30	0.47
2:B:150:VAL:HG23	2:B:200:HIS:CA	2.45	0.47
1:A:22:THR:HG22	1:A:72:THR:HG22	1.97	0.47
2:B:178:LEU:C	2:B:178:LEU:CD1	2.88	0.46
1:A:4:LEU:C	1:A:4:LEU:HD23	2.41	0.46
1:A:77:THR:HG23	1:A:77:THR:O	2.16	0.46
1:A:39:LYS:O	1:A:39:LYS:HG3	2.14	0.46
1:A:49:TYR:CE1	2:B:100(J):PRO:HB3	2.50	0.46
2:B:13:LYS:HG2	2:B:113:SER:HA	1.97	0.46
2:B:163:VAL:HA	2:B:182:VAL:HA	1.98	0.45
2:B:186:SER:HB2	2:B:187:SER:H	1.59	0.45
2:B:160:THR:O	2:B:163:VAL:CG2	2.64	0.45
2:B:40:PRO:HA	2:B:88:ALA:HB2	1.98	0.45
2:B:121:VAL:HG12	2:B:209:LYS:HG2	1.98	0.45
1:A:54:LEU:HD21	1:A:58:VAL:HB	1.97	0.45
1:A:9:SER:O	1:A:10:SER:HB2	2.17	0.45
2:B:6:GLU:HB3	2:B:107:ILE:CG2	2.46	0.45
2:B:134:GLY:HA3	2:B:186:SER:OG	2.16	0.45
2:B:38:ARG:HD3	2:B:48:LEU:HD21	1.99	0.45
2:B:160:THR:O	2:B:163:VAL:HG23	2.16	0.45
2:B:6:GLU:CB	2:B:107:ILE:HG22	2.47	0.45
2:B:95:ARG:HG2	2:B:96:ARG:N	2.30	0.45
1:A:193:GLU:HB2	1:A:206:THR:CG2	2.47	0.45
2:B:38:ARG:HD2	2:B:90:TYR:CZ	2.52	0.44
3:P:5:ASP:OD1	3:P:6:LYS:N	2.50	0.44
1:A:13:ALA:O	1:A:83:PHE:HE1	2.00	0.44
2:B:126:PRO:HB2	2:B:213:PRO:HG3	1.99	0.44
2:B:209:LYS:O	2:B:209:LYS:HG3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD12	2:B:4:LEU:N	2.33	0.44
2:B:33:GLY:O	2:B:34:VAL:C	2.60	0.44
2:B:83:SER:HG	2:B:85:VAL:HG22	1.82	0.44
2:B:9:PRO:HA	2:B:10:PRO:HD3	1.89	0.44
2:B:34:VAL:HA	2:B:96:ARG:O	2.18	0.44
2:B:72:ASP:C	2:B:72:ASP:OD1	2.61	0.43
1:A:43:PRO:HA	1:A:44:PRO:HD3	1.83	0.43
2:B:14:PRO:HG3	2:B:111:ILE:CG2	2.49	0.43
2:B:100(J):PRO:C	2:B:100(L):ASN:N	2.62	0.43
2:B:105:GLN:H	2:B:105:GLN:HG3	1.46	0.43
1:A:4:LEU:HD13	1:A:97:THR:HG22	1.99	0.43
1:A:92:HIS:CE1	3:P:8:ALA:HB1	2.54	0.43
2:B:163:VAL:O	2:B:164:HIS:CG	2.71	0.43
2:B:185:PRO:O	2:B:186:SER:C	2.61	0.43
1:A:37:ARG:HB2	1:A:86:TYR:CE2	2.53	0.43
3:P:2:LEU:CD2	3:P:3:GLU:N	2.81	0.43
1:A:13:ALA:O	1:A:83:PHE:CE1	2.72	0.43
1:A:39:LYS:O	1:A:39:LYS:CG	2.66	0.43
1:A:140:TYR:CG	1:A:141:PRO:HA	2.53	0.43
3:P:3:GLU:OE1	3:P:4:LEU:O	2.36	0.43
2:B:156:SER:HA	2:B:197:ASN:OD1	2.19	0.43
2:B:115:SER:O	2:B:116:THR:C	2.60	0.43
1:A:39:LYS:O	1:A:40:PRO:C	2.60	0.42
1:A:150:VAL:HG12	1:A:189:HIS:HB3	2.01	0.42
1:A:201:LEU:HD13	1:A:205:VAL:CG1	2.48	0.42
2:B:6:GLU:HB3	2:B:107:ILE:HG22	2.00	0.42
1:A:2:LEU:HD22	1:A:90:GLN:CD	2.43	0.42
1:A:34:ALA:O	1:A:88:CYS:HA	2.19	0.42
2:B:124:LEU:O	2:B:138:LEU:HA	2.19	0.42
2:B:203:SER:O	2:B:204:ASN:HB2	2.20	0.42
1:A:49:TYR:O	1:A:53:SER:HB2	2.20	0.42
1:A:61:ARG:NE	1:A:79:ARG:HG2	2.34	0.42
2:B:156:SER:N	2:B:197:ASN:OD1	2.50	0.42
1:A:29:VAL:O	1:A:30:THR:C	2.62	0.42
1:A:132:VAL:HG22	1:A:148:TRP:CZ3	2.55	0.42
1:A:47:LEU:HA	1:A:58:VAL:HG21	2.02	0.41
1:A:125:LEU:O	1:A:183:LYS:CD	2.55	0.41
2:B:197:ASN:ND2	2:B:208:ASP:OD1	2.48	0.41
2:B:201:LYS:N	2:B:202:PRO:CD	2.83	0.41
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.93	0.41
2:B:100(I):GLY:N	2:B:100(J):PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:2:LEU:HG	3:P:3:GLU:H	1.79	0.41
1:A:94:TYR:CE2	3:P:5:ASP:HA	2.56	0.41
2:B:195:THR:HG23	2:B:209:LYS:C	2.45	0.41
1:A:2:LEU:HD13	1:A:93:PHE:HD2	1.86	0.41
1:A:6:GLN:NE2	1:A:102:THR:CB	2.84	0.41
1:A:149:LYS:HB2	1:A:193:GLU:HG3	2.02	0.41
2:B:75:LYS:HB2	2:B:77:GLN:HG3	2.02	0.41
2:B:82(B):ARG:CG	2:B:82(B):ARG:O	2.69	0.41
2:B:186:SER:O	2:B:189:LEU:N	2.32	0.41
2:B:97:GLY:CA	2:B:100(K):VAL:HG12	2.51	0.40
2:B:148:GLU:HA	2:B:149:PRO:HA	1.94	0.40
1:A:27:GLN:HE21	1:A:27:GLN:HB2	1.65	0.40
1:A:49:TYR:CZ	1:A:53:SER:HB3	2.56	0.40
2:B:125:ALA:CB	2:B:126:PRO:CD	2.94	0.40
1:A:4:LEU:HD21	1:A:88:CYS:SG	2.61	0.40
2:B:195:THR:OG1	2:B:210:ARG:HB2	2.22	0.40
2:B:6:GLU:OE2	2:B:104:GLY:HA3	2.21	0.40
2:B:35(A):VAL:HA	2:B:93:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/214 (99%)	188 (89%)	14 (7%)	9 (4%)	2	20
2	B	210/235 (89%)	174 (83%)	25 (12%)	11 (5%)	1	17
3	P	5/13 (38%)	4 (80%)	1 (20%)	0	100	100
All	All	426/462 (92%)	366 (86%)	40 (9%)	20 (5%)	2	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	8	PRO
1	A	10	SER
2	B	15	THR
2	B	16	GLN
2	B	34	VAL
2	B	96	ARG
2	B	100(M)	ALA
2	B	186	SER
2	B	187	SER
1	A	4	LEU
1	A	40	PRO
1	A	127	SER
1	A	138	ASN
1	A	211	ARG
2	B	82(B)	ARG
2	B	112	SER
1	A	125	LEU
2	B	185	PRO
2	B	100(J)	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/187 (100%)	158 (85%)	28 (15%)	3	16
2	B	189/204 (93%)	153 (81%)	36 (19%)	1	10
3	P	6/12 (50%)	4 (67%)	2 (33%)	0	2
All	All	381/403 (94%)	315 (83%)	66 (17%)	2	12

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	LEU
1	A	11	LEU

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Mol	Chain	Res	Type
1	A	18	ARG
1	A	27	GLN
1	A	33	LEU
1	A	40	PRO
1	A	42	SER
1	A	54	LEU
1	A	73	LEU
1	A	78	LEU
1	A	81	GLU
1	A	90	GLN
1	A	122	ASP
1	A	129	THR
1	A	132	VAL
1	A	133	VAL
1	A	145	LYS
1	A	152	ASN
1	A	163	VAL
1	A	190	LYS
1	A	191	VAL
1	A	199	GLN
1	A	201	LEU
1	A	203	SER
1	A	205	VAL
1	A	208	SER
1	A	213	GLU
2	B	3	THR
2	B	4	LEU
2	B	5	LYS
2	B	7	SER
2	B	13	LYS
2	B	21	THR
2	B	25	SER
2	B	29	LEU
2	B	50	ILE
2	B	55	ASP
2	B	56	ASP
2	B	57	LYS
2	B	63	LEU
2	B	74	SER
2	B	75	LYS
2	B	77	GLN
2	B	79	VAL

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Mol	Chain	Res	Type
2	B	105	GLN
2	B	107	ILE
2	B	108	THR
2	B	115	SER
2	B	117	LYS
2	B	138	LEU
2	B	149	PRO
2	B	150	VAL
2	B	156	SER
2	B	159	LEU
2	B	163	VAL
2	B	178	LEU
2	B	183	THR
2	B	186	SER
2	B	187	SER
2	B	193	THR
2	B	209	LYS
2	B	210	ARG
2	B	212	GLU
3	P	2	LEU
3	P	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	6	GLN
1	A	27	GLN
1	A	38	GLN
1	A	90	GLN
1	A	92	HIS
1	A	138	ASN
1	A	147	GLN
1	A	152	ASN
2	B	16	GLN
2	B	39	GLN
2	B	64	ASN
2	B	77	GLN
2	B	164	HIS
2	B	192	GLN
2	B	199	ASN
2	B	204	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/214 (99%)	0.04	1 (0%) 87 72	21, 31, 44, 60	0
2	B	216/235 (91%)	0.17	2 (0%) 81 62	23, 36, 52, 59	0
3	P	7/13 (53%)	1.05	0 100 100	13, 26, 35, 46	0
All	All	436/462 (94%)	0.12	3 (0%) 84 67	13, 33, 51, 60	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	GLU	2.7
2	B	100(I)	GLY	2.6
2	B	106	GLY	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.